

Chem 505
Physical Inorganic Chemistry
Fall 2022

Instructor: Aaron Sadow, 2101B Hach Hall, Email: sadow@iastate.edu; phone: 4-8069
Class Hours: Monday, Wednesday, Friday 8:50 – 9:40 am in 2140 Hach Hall
Office Hours: MWF 9:40 am or by appointment
Required Texts: F. A. Cotton, *Chemical Applications of Group Theory*, Wiley, 1990 and Harris and Bertolucci, *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover Books

Class Goals: Learn about chemical models for molecular spectroscopy and bonding; become comfortable with anticipating molecules' structures, analyzing bonding and electronic properties in molecules, and interpreting some spectra with respect to structure and bonding.

Topics:

- (1) VSEPR, electron counting, electronic structure
- (2) Chapter 2: Properties of Groups
- (3) Chapter 3: Symmetry operations and point groups
- (4) Chapter 4: Representation of Groups
- (5) Chapter 5: Group Theory and Quantum Mechanics
- (6) Chapter 6: Symmetry Adapted Linear Combinations
- (7) Chapter 10: Molecular Vibrations
- (8) Chapter 7: MO Theory in Organic Chemistry
- (9) Chapter 8: MO Inorganic and Organometallics
- (10) Chapter 9: Ligand Field Theory and Electronic Spectroscopy
- (11) NMR spectroscopy
- (12) EPR spectroscopy

Success in the course:

Group theory and its applications in molecular orbital theory and spectroscopy require significant study efforts to understand both theoretical/abstract concepts be able to perform practical applications in analysis.

We have high standards for the class

Reading materials and practice problems should be studied prior to class.

Engage in class activities - ask questions and come prepared.

Communicate in appropriate style and language.

Punctually attend class. Excuses create embarrassment.

Do not cheat. Academic misconduct will not be tolerated.

Supplementary Literature: It is often useful to read a number of perspectives describing a topic for better understanding, and these supplementary literature are useful for that purpose.

- 1) *Molecular Symmetry and Group Theory*, Robert L. Carter, Wiley 1998
- 2) *Physical Methods in Chemistry*, R. Drago
- 3) *Introduction to Ligand Field Theory*, B. N. Figgis

Course Grading:	Two exams:	2×100 points	TBD
	Final	150 points	
	In class presentations	150 points	

Problem sets will be due before classes and reviewed in class.

Any student who may need an accommodation based on the impact of a disability should meet privately with me at the beginning of the semester to discuss specific needs. The Disability Resources Office (room 1076, Student Services Building, phone 515-294-7220 or email disabilityresources@iastate.edu) can provide more information and help coordinate reasonable accommodations for students with documented disabilities.

Content Expectations:

- (1) VSEPR. Be able to use the VSEPR approach to quickly identify simple molecular geometries as a starting point for more detailed analysis. Know how to use the periodic table to count valence shell electrons, and then apply the VSEPR scheme.
- (2) Properties of Groups: Understand what makes a Group. Matrix manipulations, multiplication rules and other operations, orders of groups, Abelian groups, classes
- (3) Symmetry Operations: Operations (identity, rotation, reflection), their representations, multiplication, point groups, assigning molecules to point groups
- (4) Orthogonality and character tables; derivation, reducing representations, projection operators
- (5) Group theory and vibrational spectroscopy. Application of projection operators to determine normal modes. Force constant analysis. Spectral analysis.
- (6) Quantum mechanics, understand how quantum mechanics is simplified by group theory. perturbation theory.
- (7) Molecular Orbital Theory: group theory and other bonding models; symmetry of the secular determinant, organic and inorganic molecular orbital diagrams.
- (8) Apply Crystal Field Theory and Ligand Field theory to understanding electronic spectra of transition metal compounds.
- (9) Other topics: Jahn-Teller Effects, crystallographic symmetry, NMR spectroscopy, EPR spectroscopy